

Hubbard Model and Lüscher fermions

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We discuss numerical complexity of the Lüscher algorithm applied to the Hubbard Model. In particular we present comparison to a certain algorithm, based on direct computation of the fermionic determinant.

1. Introduction

Recently a new type of algorithms for numerical simulations of models with dynamical fermions has been proposed by M. Lüscher [1]. The idea is based on the approximation of a fermionic determinant by the path integral over some number of bosonic fields, which allows ones to elegantly avoid the main difficulty coming from the nonlocality of the fermionic determinant. The complexity of a sweep of the Lüscher algorithm is proportional to the volume of the system and in this respect it wins in comparison with the standard hybrid Monte Carlo [2]. Of course, what is interesting in practice is a comparison of the computer cost needed to produce independent configurations which is the product of the sweep cost and the autocorrelation time. Therefore the crucial question is how the autocorrelation time depends on the volume of the system. Contrary to the sweep time the autocorrelation time can strongly depend on the external parameters. Therefore it is particularly interesting to test the dependence of the autocorrelation time on the various interesting physical parameters. Recent results obtained in QCD are rather promising showing that the computational cost needed to obtain independent configurations is comparable to the standard HMC algorithms [3].

In this letter we present new results of numerical simulations of the Hubbard Model using the Lüscher method and compare them to standard methods in context of the algorithmical complexity. This is a continuation of our contribution to the proceedings Lattice 95 where we presented preliminary results [4]. In particular, we noted

there possible improvements which reduce autocorrelation times. Here, we study the errors introduced by the bosonic approximation and compare dynamical properties of the multiboson algorithm with the simple exact algorithm.

2. Lüscher approximation

We consider the Hubbard Model defined by the Hamiltonian

$$\mathcal{H} = -K \sum_{\langle ij \rangle \sigma} a_{i\sigma}^\dagger a_{j\sigma} - \frac{U}{2} \sum_i (n_{i\uparrow} - n_{i\downarrow})^2 \quad (1)$$

where $a_{i\sigma}$ are fermionic operators acting on electrons on site i of the lattice. The sum runs over nearest neighbors (each symmetric pair $\langle i, j \rangle$ is counted twice). Physical parameters entering the model are: K - hopping parameter, U - the strength of the effective Coulomb interaction, and the inverse temperature β . The interaction term of the Hamiltonian describes the system with the half-filled band. One find the following representation of the partition function for the model [5] :

$$Z \simeq \int [dAd\phi] \exp \left(- \int A^2(x)/2 \, d^3x \right) \exp \left(- \int \sum_{k=1}^n \phi_k^\dagger [(\mathcal{Q}^\dagger \mathcal{Q} - \alpha_k)^2 + \beta_k^2] \phi_k d^3x \right) \quad (2)$$

where $\mathcal{Q}^\dagger \mathcal{Q} \equiv \mathcal{M}^\dagger \mathcal{M} / \lambda_{max}$ and λ_{max} denotes the largest eigenvalue of the matrix $\mathcal{M}^\dagger \mathcal{M}$. The matrix \mathcal{M} is the fermion matrix entering the Euclidean formulation

$$\Psi^* \mathcal{M} \Psi = \frac{K\beta}{N_t} \sum_{\langle ij \rangle t} \Psi_{it}^* \Psi_{jt} + \sum_{it} \Psi_{it}^* (\Psi_{it} - \Psi_{it-1})$$

$$+ \sum_{it} \Psi_{it}^* \Psi_{it} \left(\exp \left[\sqrt{\frac{U\beta}{N_t}} A_{it} - \frac{U\beta}{N_t} \right] - 1 \right).$$

$A(x)$ is the Hubbard-Stratanovich continuous field, and $\phi_k(x)$ are the auxiliary bosonic fields. The particular form of the polynomial $P_n(x)$ used in the approximation of the function $1/x$, is built from the Chebyshev polynomials and gives a rapid uniform convergence to the function $1/x$ in the interval $(\epsilon, 1)$. Its roots are introduced already in (2) and their real and imaginary parts are denoted by $\alpha_k + i\beta_k, k = 1, \dots, n$ respectively. The relative error of the approximation defined as $|R(x)| = |xP_n(x) - 1|$ is exponentially bounded

$$|R(x)| < 2 \left(\frac{1 - \sqrt{\epsilon}}{1 + \sqrt{\epsilon}} \right)^{n+1}. \quad (3)$$

One sees that to decrease ϵ one has to increase n . The most economic choice of ϵ corresponds to the largest possible value which still gives a good approximation of the determinant. To make this statement precise we introduce following the quantity [6] as a measure of error (or goodness)

$$\delta = |y^{1/V} - 1| \quad (4)$$

where

$$y = \det(Q^\dagger Q) P_n(Q^\dagger Q). \quad (5)$$

The power $1/V$, where V is naturally adjusted to the dimension of the matrix \mathcal{M} . Figure 1 shows δ as a function of ϵ for a different numbers of fields measured on a one typical configuration. The optimal value of ϵ lies close to the smallest eigenvalue of the matrix $Q^\dagger Q$ ($\lambda_{min} = 0.032$). Such a behavior is consistent with the previous findings in the QCD case.

3. Exact algorithm

To compare the computational cost of the multiboson algorithm with the cost of the more standard approaches, we implemented a simple exact algorithm based on the updating scheme allowing for computing changes in the matrix \mathcal{M}^{-1} while making trial changes in the matrix \mathcal{M} . In order to update the field A located on the site i one must calculate the ratio of the fermion determinants. Since the only A dependent elements of

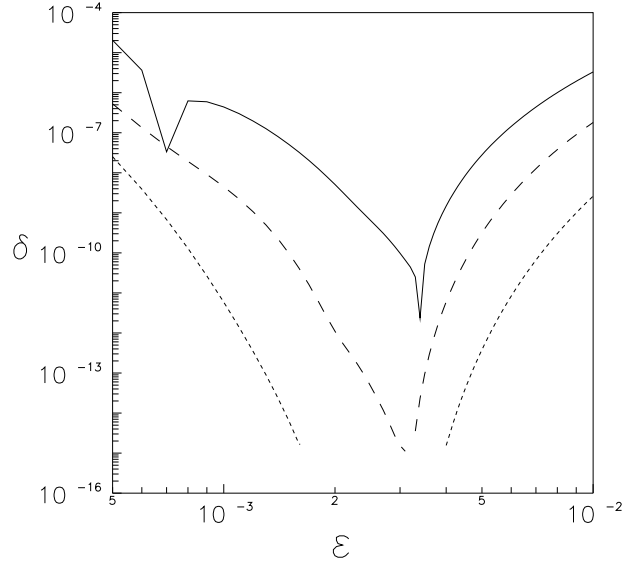


Figure 1. Errors of the Lüscher approximation measured on a single typical configuration. The quantity δ defined in text is shown as a function of ϵ . The solid, dashed and dotted line is for number of fields 50, 70 and 100 respectively

the matrix \mathcal{M} lie on the diagonal we consider the following change in the matrix \mathcal{M} ,

$$\mathcal{M}' = (I + \Delta)\mathcal{M}, \quad (6)$$

where Δ is matrix with one nonzero element $\Delta_{ij} = \delta_{ij}d$. Then

$$\frac{\det \mathcal{M}'}{\det \mathcal{M}} = \det(I + \mathcal{M}^{-1}\Delta) = 1 + \mathcal{M}_{ii}^{-1}d \quad (7)$$

is determined completely by elements of the matrix \mathcal{M}^{-1} . Once the trial change has been accepted the updated matrix \mathcal{M}^{-1} can be evaluated from the formula

$$\mathcal{M}'^{-1} = \mathcal{M}^{-1} - \frac{\mathcal{M}^{-1}\Delta\mathcal{M}^{-1}}{1 + d\mathcal{M}_{ii}^{-1}}. \quad (8)$$

This process is very economical from the computational point of view since one update of \mathcal{M}^{-1} requires $O(V^2)$ operations comparing with $O(V^3)$ operations needed to evaluate the determinant with the brute force method. Also the today's leading algorithm for simulations of the Hubbard

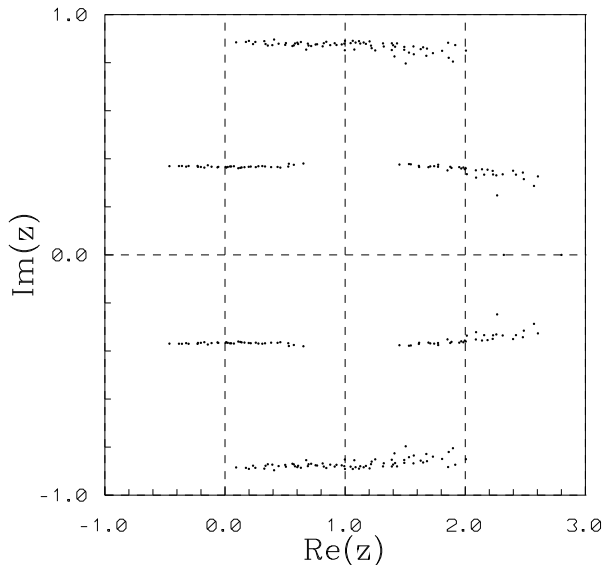


Figure 2. Eigenvalues of the matrix \mathcal{M} on the complex plane

Model is essentially based on it [7]. However, contrary to the standard one our particular formulation of path integrals does not require multiplication badly conditioned matrices. Thus we believe that this is free of the numerical instabilities. Indeed, we performed thousands sweeps at β up to 8 without accumulating numerical errors. An additional cost comes from working with larger matrices.

4. Final remarks

As we have previously reported the strong autocorrelation between generated configurations is a serious obstacle which limits the available range of parameters to $U \leq 2$ and $\beta = 1$ for the multi-boson algorithm. In contrast the program based on exact evaluation of the fermionic determinant has no such restrictions and works equally good at $U = 1$ and $U = 4$.

The comparison of CPU time needed for both algorithms varies accordingly to the lattice sizes. On small lattices exact algorithm is substantially faster. For example for a lattice $6^2 \times 8$ in our experiments on the workstation HP735/125 it takes 20 minutes which should be compared with 10 hours

needed for our implementation of the Lüscher algorithm to produce results of the same quality. Of course for larger lattices the computational cost grows much more faster for the exact algorithm. In the region of weak coupling we were able to could simulate with the Lüscher algorithm lattices with the size up to $16^2 \times 8$.

The polynomial approximation of the function $1/x$ can be extended to the complex plane [8]. Thus one try to approximate directly the inverse of the matrix \mathcal{M} . This would reduce the condition numbers for matrices entering the problem and would result in the simpler final action. This modification of the original Lüscher idea gave very promising results [9]. However, in contrast to the QCD case the matrix \mathcal{M} for the Hubbard Model has eigenvalues with the positive and negative real parts as can for example be seen in Figure 2. Because one cannot extend the domain of the convergence beyond the singular point (0,0), this is, unfortunately, impossible to adopt this modification to the Hubbard Model.

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